

BOUNDS FOR THE DISTANCE ESTRADA INDEX OF GRAPHS

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Abstract

The D -eigenvalues $\mu_1, \mu_2, \dots, \mu_n$ of a connected graph G are the eigenvalues of its distance matrix. The distance Estrada index of G is defined in [15] as

$$DEE = DEE(G) = \sum_{i=1}^n e^{\mu_i}$$

In this paper, we give better lower bounds for the distance Estrada index of any connected graph as well as some relations between $DEE(G)$ and the distance energy.

Keywords: Distance energy, Distance Estrada index, Bound.

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1 Introduction

Let G be a simple connected graph with n vertices and m edges on vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. Throughout this paper, such a graph will be referred to as connected (n, m) -graph. The distance matrix $D = D(G)$ of G is defined so that its (i, j) -entry is equal to $d_G(v_i, v_j)$, denoted by d_{ij} , the distance (i.e., the length of the shortest path [1]) between the vertices v_i and v_j of G . The diameter of the graph G is the maximum distance between any two vertices of G . Let Δ be diameter of G and $A(G)$ be the adjacency matrix of G . The eigenvalues of $A(G)$ are called the eigenvalues of G and the eigenvalues of $D(G)$ are said to be the D -eigenvalues of G [2]. Since $A(G)$ and $D(G)$ are real symmetric matrices their eigenvalues are real numbers. So we can order them so that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ and $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ are the eigenvalues and D -eigenvalues of G , respectively.

The Estrada index of the graph G is defined in [4-8] as:

$$EE = EE(G) = \sum_{i=1}^n e^{\lambda_i} \quad (1)$$

The Estrada index of graphs has an important role in Chemistry and Physics. There exist a vast literature related to Estrada index and its bounds. For more information see [4-12]. Because of the evident success of the graph Estrada index, Estrada index based of the eigenvalues of other graph matrices have, one-by-one, been introduced. From this respect, the authors defined the distance Estrada index $DEE(G)$ based on distance matrix of the graph G as the following

$$DEE = DEE(G) = \sum_{i=1}^n e^{\mu_i}. \quad (2)$$

where $\mu_1, \mu_2, \dots, \mu_n$ are the D -eigenvalues of G .

Let

$$N_k = \sum_{i=1}^n (\mu_i)^k.$$

Recalling the power series expansion of e^x we have another expression of distance Estrada index as the following

$$DEE(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!}. \quad (3)$$

Some well known mathematical properties on the distance Estrada index of the graph G are established as follows:

Theorem 1.1 [15] *Let G be a connected (n, m) -graph and Δ the diameter of G . Then the distance Estrada index is bounded as follows*

$$\sqrt{n^2 + 4m} \leq DEE(G) \leq n - 1 + e^{\Delta \sqrt{n(n-1)}}. \quad (4)$$

Equality holds on both sides of (4) if and only if $G \simeq K_1$.

Theorem 1.2 [15] *Let G be a connected (n, m) -graph and Δ the diameter of G . Then*

$$DEE(G) - E_D(G) \leq n - 1 - \Delta \sqrt{n(n-1)} + e^{\Delta \sqrt{n(n-1)}} \quad (5)$$

or

$$DEE(G) \leq n - 1 + e^{E_D(G)}. \quad (6)$$

Equality holds in (5) or (6) if and only if $G \simeq K_1$.

We organize this paper in the following way. In section 2, we obtain better lower bounds for $DEE(G)$. In section 3, we give some relations between $DEE(G)$ and the distance energy.

2 Lower bounds for the distance Estrada index

In this section, we obtain some lower bounds for the distance Estrada index of any connected graph G using the same procedure in [12]. Firstly, we give the following definitions and lemmas which will be needed then.

Definition 2.1 [14] Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$ and a distance matrix D . Then the distance degree of v_i , denoted by D_i is given by $D_i = \sum_{j=1}^n d_{ij}$.

Definition 2.2 [14] Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$ and a distance matrix D . Let the distance degree sequence be $\{D_1, D_2, \dots, D_n\}$. Then the second distance degree of v_i , denoted by T_i is given by $T_i = \sum_{j=1}^n d_{ij} D_j$.

Definition 2.3 [16] Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$ and a distance matrix D . Let the distance degree sequence be $\{D_1, D_2, \dots, D_n\}$. Then for each $i = 1, 2, \dots, n$ the sequence $M_i^{(1)}, M_i^{(2)}, \dots, M_i^{(t)}, \dots$ is defined as follows: Fix $\alpha \in \mathbb{R}$, let

$$M_i^{(1)} = D_i^\alpha$$

and for each $t \geq 2$, let

$$M_i^{(t)} = \sum_{j=1}^n d_{ij} M_j^{(t-1)}.$$

Definition 2.4 [3] Let G be a graph with distance matrix D . Then the Wiener index of G , denoted by $W(G)$ is given by $W(G) = \frac{1}{2} \sum_{i=1}^n D_i$.

Lemma 2.1 [16] Let G be a connected graph α be a real number and t be an integer. Then

$$\mu_1 \geq \sqrt{\frac{S_{t+1}}{S_t}}.$$

where $S_t = \sum_{i=1}^n (M_i^{(t)})^2$. Moreover, equality holds for particular values of α and t if and only if

$$\frac{M_1^{(t+1)}}{M_1^{(t)}} = \frac{M_2^{(t+1)}}{M_2^{(t)}} = \dots = \frac{M_n^{(t+1)}}{M_n^{(t)}}.$$

Lemma 2.2 [14] A connected graph G has two distinct D -eigenvalues if and only if G is a complete graph.

Lemma 2.3 [17] *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$\mu_1 \geq 2(n-1) - \frac{2m}{n}$$

with equality if and only if $G = K_n$ or G is a regular graph of diameter two.

Now we are ready to give the main results of this section.

Theorem 2.1 *Let G be a connected (n, m) -graph. Then*

$$DEE(G) \geq e^{\sqrt{\frac{S_{t+1}}{S_t}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{S_{t+1}}{S_t}}}}. \quad (7)$$

where α is a real number, t is an integer and $S_t = \sum_{i=1}^n \left(M_i^{(t)}\right)^2$. Moreover, the equality holds in (7) if and only if G is the complete graph K_n .

Proof. Starting with the equation (2) and using Arithmetic-Geometric Mean Inequality, we get

$$\begin{aligned} DEE(G) &= e^{\mu_1} + e^{\mu_2} + \dots + e^{\mu_n} \\ &\geq e^{\mu_1} + (n-1) \left(\prod_{i=2}^n e^{\mu_i} \right)^{\frac{1}{n-1}} \end{aligned} \quad (8)$$

$$= e^{\mu_1} + (n-1) \left(e^{-\mu_1} \right)^{\frac{1}{n-1}}, \text{ since } \sum_{i=1}^n \mu_i = 0. \quad (9)$$

Consider the following function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}}$$

for $x > 0$. We have

$$f'(x) = e^x - e^{-\frac{x}{n-1}} > 0$$

for $x > 0$. It is easy to see that f is an increasing function for $x > 0$. From the equation (9) and Lemma 2.1, we obtain

$$DEE(G) \geq e^{\sqrt{\frac{S_{t+1}}{S_t}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{S_{t+1}}{S_t}}}}. \quad (10)$$

This completes the first part of the proof.

Now we suppose that the equality holds in (7). Then all inequalities in the above argument must be equalities. From (10) we have

$$\mu_1 = \sqrt{\frac{S_{t+1}}{S_t}}$$

which implies $\frac{M_1^{(t+1)}}{M_1^{(t)}} = \frac{M_2^{(t+1)}}{M_2^{(t)}} = \dots = \frac{M_n^{(t+1)}}{M_n^{(t)}}$. From (8) and Arithmetic-Geometric Mean Inequality we get $\mu_2 = \mu_3 = \dots = \mu_n$. Therefore G has exactly two distinct D -eigenvalues, by Lemma 2.2, G is the complete graph K_n .

Conversely, one can easily see that the equality holds in (7) for the complete graph K_n . This completes the proof.

The following result states a lower bound for the distance Estrada index involving Wiener index.

Corollary 2.1 *Let G be a connected (n, m) -graph. Then*

$$DEE(G) \geq e^{\frac{2W(G)}{n}} + \frac{n-1}{e^{\frac{2W(G)}{n(n-1)}}} \quad (11)$$

where $W(G)$ denotes the Wiener index of the graph G . Moreover the equality holds in (11) if and only if G is the complete graph K_n .

Proof. In [16], Güngör and Bozkurt showed that the following inequality (see Theorem 2)

$$\mu_1 \geq \sqrt{\frac{S_{t+1}}{S_t}} \geq \sqrt{\frac{\sum_{i=1}^n T_i^2}{\sum_{i=1}^n D_i^2}}. \quad (12)$$

where $S_t = \sum_{i=1}^n \left(M_i^{(t)}\right)^2$. Also in [14], Indulal proved the following result using Cauchy-Schwartz inequality (see Theorem 4)

$$\mu_1 \geq \sqrt{\frac{\sum_{i=1}^n T_i^2}{\sum_{i=1}^n D_i^2}} \geq \sqrt{\frac{\sum_{i=1}^n D_i^2}{n}} \geq \frac{2W(G)}{n}. \quad (13)$$

Combining Theorem 2.1, (12) and (13) we get the inequality (11).

Also, the equality holds in (11) if and only if G is the complete graph K_n .

Theorem 2.2 *Let G be a connected (n, m) -graph with $n \geq 2$ vertices. Then*

$$DEE(G) \geq e^{2(n-1)-\frac{2m}{n}} + e^{-(2(n-1)-\frac{2m}{n})} + n - 2. \quad (14)$$

Moreover the equality holds in (14) if and only if $G = K_2$.

Proof. Since G is a connected graph $\mu_1 > 0$ and $\mu_n < 0$. Now

$$\begin{aligned} DEE(G) &= e^{\mu_1} + e^{\mu_2} + \dots + e^{\mu_n} \\ &\geq e^{\mu_1} + e^{\mu_n} + (n-2) \left(\prod_{i=2}^{n-1} e^{\mu_i} \right)^{\frac{1}{n-2}} \end{aligned} \quad (15)$$

$$= e^{\mu_1} + e^{\mu_n} + (n-2)e^{-\frac{\mu_1 + \mu_n}{n-2}}, \text{ since } \sum_{i=1}^n \mu_i = 0. \quad (16)$$

We consider the following function

$$f(x, y) = e^x + e^y + (n-2)e^{-\frac{x+y}{n-2}}$$

for $x > 0, y < 0$. In [12], Das and Lee showed that $f(x, y)$ has a minimum value at $x + y = 0$ and its minimum value is $e^x + e^{-x} + n - 2$ (see Theorem 2.4). Also we can easily see that $e^x + e^{-x} + n - 2$ is an increasing function for $x > 0$. By Lemma 2.3 we obtain

$$e^{\mu_1} + e^{-\mu_1} + n - 2 \geq e^{2(n-1)-\frac{2m}{n}} + e^{-(2(n-1)-\frac{2m}{n})} + n - 2. \quad (17)$$

From the equation (16) and (17), we get

$$DEE(G) \geq e^{2(n-1)-\frac{2m}{n}} + e^{-(2(n-1)-\frac{2m}{n})} + n - 2.$$

This completes the first part of the theorem.

Now we suppose that the equality holds in (14). Then all inequalities in the above argument must be equalities. Since $\mu_1 + \mu_n = 0$, we have that $-\mu_1$ is also an D -eigenvalue of G . From equality in (17) and Lemma 2.3 we can write G is the complete graph K_n . From equality in (15) and $\sum_{i=1}^n \mu_i = 0$ we obtain

$$\mu_2 = \mu_3 = \dots = \mu_{n-1} = 0$$

since $\mu_1 + \mu_n = 0$. In [17], Zhou and Trinajstić showed that this situation is not valid for $n \geq 3$ (see Theorem 4). Therefore the equality holds in (14) for only the graph $G = K_2$.

Conversely, one can easily see that the equality holds in (14) for the complete graph K_2 . This completes the proof.

3 Bounds for the distance Estrada index involving the distance energy

In this section, we firstly recall the distance energy $E_D(G)$ which is defined in [13] as

$$E_D(G) = \sum_{i=1}^n |\mu_i| \quad (18)$$

where $\mu_1, \mu_2, \dots, \mu_n$ are the D -eigenvalues of G .

Now, we will adapt the some results in [10] on distance Estrada index to give some relations between the distance Estrada index $DEE(G)$ and the distance energy $E_D(G)$.

Theorem 3.1 *Let G be a connected (n, m) -graph. Then the distance Estrada index $DEE(G)$ and the distance energy $E_D(G)$ satisfy the following inequality*

$$\frac{1}{2}E_D(G)(e-1) + n - n_+ \leq DEE(G) \leq n - 1 + e^{\frac{E_D(G)}{2}}. \quad (19)$$

where n_+ denotes the number of positive D -eigenvalues of G . Moreover, the equality holds on both sides of (19) if and only if $G = K_1$.

Proof. Lower bound: Since $e^x \geq ex$, equality holds if and only if $x = 1$ and $e^x \geq 1 + x$, equality holds if and only if $x = 0$. We get

$$\begin{aligned} DEE(G) &= \sum_{i=1}^n e^{\mu_i} = \sum_{\mu_i > 0} e^{\mu_i} + \sum_{\mu_i \leq 0} e^{\mu_i} \\ &\geq \sum_{\mu_i > 0} e\mu_i + \sum_{\mu_i \leq 0} (1 + \mu_i) \\ &= e(\mu_1 + \mu_2 + \dots + \mu_{n_+}) + (n - n_+) + (\mu_{n_++1} + \dots + \mu_n) \\ &= (e-1)(\mu_1 + \mu_2 + \dots + \mu_{n_+}) + (n - n_+) + \sum_{i=1}^n \mu_i \\ &= \frac{1}{2}E_D(G)(e-1) + n - n_+. \end{aligned}$$

Upper bound: Since $f(x) = e^x$ monotonically increases in the interval

$(-\infty, +\infty)$, we obtain

$$\begin{aligned}
DEE(G) &= \sum_{i=1}^n e^{\mu_i} \leq n - n_+ + \sum_{i=1}^{n_+} e^{\mu_i} \\
&= n - n_+ + \sum_{i=1}^{n_+} \sum_{k \geq 0} \frac{(\mu_i)^k}{k!} \\
&= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\mu_i)^k
\end{aligned}$$

and

$$\begin{aligned}
DEE(G) &\leq n + \sum_{k \geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n_+} (\mu_i) \right]^k \\
&= n - 1 + e^{\frac{E_D(G)}{2}}.
\end{aligned}$$

It is easy to see that the equality holds on both sides of (19) if and only if $E_D(G) = 0$. Since G is a connected graph this only happens in the case of $G = K_1$.

Remark 3.1 It is clear that the upper bound in (19) is better than the upper bound in (6). Moreover, the lower bounds in (7), (14) and (19) are nicer than the lower bound (4). For instance, let G be the path graph P_4 . Then the bounds in (7) (when $\alpha = 1$ and $t = 2$), (14), (19) and (4) give $DEE(P_4) \geq 175.069$, $DEE(P_4) \geq 92.028$, $DEE(P_4) \geq 11.870$ and $DEE(P_4) \geq 5.291$, respectively. Although the best lower bound of this study is the lower bound in (7), we think that readers like using the lower bound in (14) for practical purposes.

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